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Dichlorido(dimethyl sulfoxide-κO)(1,10-phenanthroline-5,6-dione-$\kappa^2 N,N'$)-copper(II) dimethyl sulfoxide monohydrate

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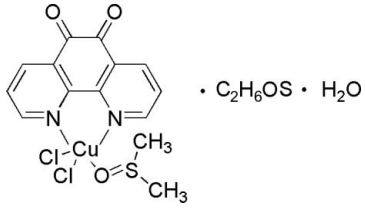
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.039; wR factor = 0.121; data-to-parameter ratio = 14.8.

The title compound, $[CuCl_2(C_{12}H_6N_2O_2)(C_2H_6OS)]\cdot C_2H_6OS\cdot H_2O$, was obtained by the reaction of 1,10-phenanthroline-5,6-dione (phendione) and $CuCl_2\cdot 2H_2O$. The copper(II) ion is pentacoordinated in a distorted square-pyramidal environment. The water molecule connects the complex and a dimethyl sulfoxide solvent molecule by O—H···O and O—H···Cl hydrogen bonds.

Related literature

For related literature, see: Addison & Rao (1984); Coyle *et al.* (2003); Deegan *et al.* (2006); Eshwika *et al.* (2004); Ghosh *et al.* (2006); Xu *et al.* (2006); Yamada *et al.* (1992).



Experimental

Crystal data

$[CuCl_2(C_{12}H_6N_2O_2)(C_2H_6OS)]\cdot C_2H_6OS\cdot H_2O$
M_r = 518.90
Triclinic, $P\overline{1}$
a = 7.213 (2) Å
b = 13.285 (4) Å
c = 13.316 (4) Å
α = 61.405 (4)°
β = 76.169 (5)°
γ = 86.688 (5)°
V = 1085.5 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.47 mm^{-1}
T = 293 (2) K
0.30 × 0.20 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.654, T_{max} = 1.000
(expected range = 0.532–0.814)
5536 measured reflections
3809 independent reflections
2886 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.121
S = 1.04
3809 reflections
257 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O4	0.97	2.15	3.037 (5)	151
O5—H5B···Cl2^{i}	0.91	2.38	3.233 (5)	158

Symmetry code: (i) $x, y+1, z$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2463).

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supplementary materials

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Dichlorido(dimethyl sulfoxide-κO)(1,10-phenanthroline-5,6-dione-$\kappa^2 N,N'$)copper(II) dimethyl sulfoxide monohydrate

G.-J. Xu, M.-J. Xie, L. Feng, S.-P. Yan and D.-Z. Liao

Comment

The complexes of 1,10-phenanthroline-5,6-dione (phendione) could intercalate within the base pairs of DNA (Ghosh *et al.*, 2006; Coyle *et al.*, 2003). Based on this finding, the derivatives of phendione are promising in the treatment of many diseases (Deegan *et al.*, 2006; Eshwika *et al.*, 2004), cancer amongst all, and their development is still in progress. Following our interest in biological activity of metal complexes, we decided to focus our attention on the complexes of phendione (Xu *et al.*, 2006).

The asymmetric unit of complex consists of a monomeric copper(II) complex, one dimethyl sulfoxide (DMSO) molecule and one water molecule. The copper(II) ion is in a five-coordinated environment. The phendione acts as bidentate ligand [Cu—N1 = 2.062 (3)Å and Cu—N2 = 2.059 (3) Å], forming with the metal ion a five-membered chelate ring with a bite angle of 80.38 (12)°. A monodentate dimethyl sulfoxide interacts with copper at a distance [Cu—O3 = 2.019 (3) Å]. Addison *et al.* (1984) have proposed a structural index for five-coordinated geometries of copper(II). This index has been defined as $\tau = (\beta-\alpha)/60$, with β and α being the two largest angles. For perfect tetragonal geometry τ equals zero, while it becomes unity for perfect trigonal bipyramidal geometry. From the bond lengths and angles it can be concluded that the coordination geometry around copper(II) is clearly square-pyramidal ($\tau = 0.14$) with a CuN_2OCl plane and one chloride ion in the apex. The copper(II) ion is shifted 0.3319 Å out of the plane defined by (N1, N2, O3 and Cl1) and directed towards Cl2.

The water molecule connects the complex and a dimethyl sulfoxide solvent molecule by O—H···O and O—H···Cl hydrogen bonds.

Experimental

1,10-Phenanthroline-5,6-dione was prepared according to the literature method (Yamada *et al.*, 1992). The complex was prepared by mixing a 10 ml me thanolic solution of copper(II) chloride dihydrate (171 mg, 0.5 mmol) and 1,10-phenanthroline-5,6-dione (105 mg, 0.5 mmol) in methanolic solution (10 ml) was added, and then the solution was stirred for about 3 h at room temperature. The green precipitate was collected by filtration. Crystals of suitable quality for X-ray analysis were obtained by slow evaporation of a dimethyl sulfoxide solution.

Refinement

All H atoms were initially located in a difference Fourier map, but refined using a riding model with with C—H distances in the range 0.95–1.00 Å, O—H = 0.91 and 0.97Å and $U_{iso}(H) = 1.2U_{eq}(C,O)$. The methyl H atoms were then constrained to an ideal geometry, with C—H distances of 0.98 Å and $U_{iso}(H) = 1.5U_{eq}(C)$, but each group was allowed to rotate freely about its C—C bond.

Figures

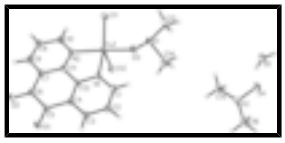


Fig. 1. Molecular view of the title complex with the atomic labeling scheme. Displacement ellipsoids are shown at the 30% probability level.

Dichlorido(dimethyl sulfoxide-κ*O*)(1,10-phenanthroline-5,6-dione-κ^2*N*,*N*')copper(II) dimethyl sulfoxide monohydrate

Crystal data

$[CuCl_2(C_{12}H_6N_2O_2)(C_2H_6OS)]\cdot C_2H_6OS\cdot H_2O$	$Z = 2$
$M_r = 518.90$	$F_{000} = 530$
Triclinic, $P\overline{1}$	$D_x = 1.588$ Mg m^{-3}
$a = 7.213$ (2) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 13.285$ (4) Å	Cell parameters from 2461 reflections
$c = 13.316$ (4) Å	$\theta = 2.9$–27.3°
$\alpha = 61.405$ (4)°	$\mu = 1.47$ mm^{-1}
$\beta = 76.169$ (5)°	$T = 293$ (2) K
$\gamma = 86.688$ (5)°	Block, green
$V = 1085.5$ (6) Å^3	0.30 × 0.20 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3809 independent reflections
Radiation source: fine-focus sealed tube	2886 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.024$
$T = 293$(2) K	$\theta_{max} = 25.0^\circ$
φ and ω scans	$\theta_{min} = 1.8^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$h = -8\rightarrow8$
$T_{min} = 0.654$, $T_{max} = 1.000$	$k = -10\rightarrow15$
5536 measured reflections	$l = -7\rightarrow15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.039$	H-atom parameters constrained
$wR(F^2) = 0.121$	$w = 1/[\sigma^2(F_o^2) + (0.0706P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$

3809 reflections	$\Delta\rho_{max}$ = 0.54 e Å^{-3}
257 parameters	$\Delta\rho_{min}$ = −0.50 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.68285 (7)	0.20517 (4)	0.11889 (4)	0.02951 (17)
Cl1	0.7899 (2)	0.32022 (10)	−0.08024 (10)	0.0523 (3)
Cl2	0.98176 (15)	0.15681 (9)	0.19795 (9)	0.0395 (3)
O1	0.1728 (5)	−0.2722 (3)	0.5060 (3)	0.0508 (9)
O2	0.3546 (5)	−0.3228 (3)	0.3314 (3)	0.0529 (9)
N1	0.4842 (5)	0.1080 (3)	0.2746 (3)	0.0283 (7)
N2	0.6593 (4)	0.0587 (3)	0.1052 (3)	0.0273 (7)
C1	0.4025 (6)	0.1372 (4)	0.3593 (4)	0.0372 (10)
H1	0.4317	0.2103	0.3465	0.045*
C2	0.2762 (6)	0.0620 (4)	0.4650 (4)	0.0405 (11)
H2	0.2214	0.0852	0.5206	0.049*
C3	0.2336 (6)	−0.0481 (4)	0.4857 (4)	0.0376 (10)
H3	0.1512	−0.0997	0.5559	0.045*
C4	0.3165 (5)	−0.0803 (3)	0.3994 (3)	0.0273 (9)
C5	0.2780 (6)	−0.1980 (4)	0.4167 (4)	0.0347 (10)
C6	0.3800 (6)	−0.2259 (4)	0.3177 (4)	0.0353 (10)
C7	0.5102 (6)	−0.1347 (3)	0.2090 (4)	0.0324 (9)
C8	0.6115 (6)	−0.1544 (4)	0.1163 (4)	0.0384 (10)
H8	0.5950	−0.2248	0.1193	0.046*
C9	0.7360 (6)	−0.0680 (4)	0.0207 (4)	0.0393 (10)
H9	0.8061	−0.0802	−0.0404	0.047*
C10	0.7550 (6)	0.0378 (4)	0.0173 (3)	0.0339 (10)
H10	0.8367	0.0960	−0.0480	0.041*
C11	0.5396 (5)	−0.0261 (3)	0.2003 (3)	0.0252 (8)
C12	0.4413 (5)	0.0007 (3)	0.2951 (3)	0.0252 (8)
S1	0.79906 (15)	0.43275 (9)	0.09613 (9)	0.0335 (3)
O3	0.6295 (4)	0.3409 (2)	0.1482 (3)	0.0374 (7)
C13	0.6938 (8)	0.5662 (4)	0.0314 (6)	0.077 (2)

H13A	0.6706	0.5795	−0.0419	0.115*
H13B	0.7790	0.6269	0.0174	0.115*
H13C	0.5750	0.5642	0.0838	0.115*
C14	0.8440 (11)	0.4352 (6)	0.2211 (5)	0.091 (2)
H14A	0.7293	0.4517	0.2632	0.137*
H14B	0.9432	0.4935	0.1953	0.137*
H14C	0.8837	0.3617	0.2720	0.137*
S2	0.63777 (15)	0.62156 (9)	0.50874 (10)	0.0376 (3)
O4	0.6473 (4)	0.7528 (2)	0.4453 (3)	0.0444 (8)
C15	0.8179 (8)	0.5835 (4)	0.4152 (5)	0.0541 (13)
H15A	0.7891	0.6132	0.3397	0.081*
H15B	0.8198	0.5014	0.4507	0.081*
H15C	0.9409	0.6157	0.4054	0.081*
C16	0.7491 (7)	0.5797 (4)	0.6291 (4)	0.0469 (12)
H16A	0.8742	0.6182	0.5997	0.070*
H16B	0.7600	0.4981	0.6666	0.070*
H16C	0.6725	0.6005	0.6852	0.070*
O5	1.0108 (5)	0.8885 (3)	0.2676 (3)	0.0571 (9)
H5A	0.9228	0.8233	0.3256	0.069*
H5B	0.9671	0.9578	0.2554	0.069*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0328 (3)	0.0211 (3)	0.0286 (3)	−0.0039 (2)	−0.0017 (2)	−0.0091 (2)
Cl1	0.0765 (9)	0.0347 (6)	0.0295 (6)	−0.0109 (6)	−0.0054 (6)	−0.0047 (5)
Cl2	0.0376 (6)	0.0404 (6)	0.0410 (6)	0.0036 (5)	−0.0108 (5)	−0.0193 (5)
O1	0.054 (2)	0.0378 (19)	0.0383 (18)	−0.0198 (16)	0.0016 (15)	−0.0044 (15)
O2	0.077 (2)	0.0281 (18)	0.054 (2)	−0.0146 (16)	−0.0163 (18)	−0.0178 (16)
N1	0.0329 (18)	0.0204 (17)	0.0331 (18)	−0.0015 (14)	−0.0035 (15)	−0.0157 (15)
N2	0.0269 (17)	0.0262 (18)	0.0246 (17)	0.0007 (14)	−0.0037 (14)	−0.0099 (15)
C1	0.042 (2)	0.029 (2)	0.040 (2)	−0.0028 (19)	−0.002 (2)	−0.020 (2)
C2	0.038 (2)	0.046 (3)	0.040 (3)	0.001 (2)	0.003 (2)	−0.028 (2)
C3	0.034 (2)	0.039 (3)	0.032 (2)	−0.002 (2)	0.0004 (19)	−0.015 (2)
C4	0.026 (2)	0.025 (2)	0.027 (2)	−0.0021 (16)	−0.0051 (16)	−0.0104 (18)
C5	0.034 (2)	0.031 (2)	0.032 (2)	−0.0051 (19)	−0.0103 (19)	−0.008 (2)
C6	0.040 (2)	0.030 (2)	0.036 (2)	−0.0036 (19)	−0.0139 (19)	−0.013 (2)
C7	0.034 (2)	0.028 (2)	0.036 (2)	−0.0004 (18)	−0.0123 (18)	−0.0138 (19)
C8	0.052 (3)	0.031 (2)	0.042 (3)	0.007 (2)	−0.016 (2)	−0.024 (2)
C9	0.044 (3)	0.043 (3)	0.032 (2)	0.008 (2)	−0.004 (2)	−0.021 (2)
C10	0.033 (2)	0.037 (2)	0.028 (2)	−0.0007 (19)	−0.0020 (18)	−0.015 (2)
C11	0.030 (2)	0.019 (2)	0.026 (2)	0.0039 (16)	−0.0087 (16)	−0.0092 (17)
C12	0.0235 (19)	0.026 (2)	0.025 (2)	0.0014 (16)	−0.0071 (16)	−0.0105 (17)
S1	0.0327 (6)	0.0236 (5)	0.0375 (6)	−0.0054 (4)	−0.0021 (5)	−0.0114 (5)
O3	0.0345 (16)	0.0251 (15)	0.0463 (17)	−0.0071 (12)	0.0030 (13)	−0.0170 (14)
C13	0.051 (3)	0.021 (3)	0.127 (6)	−0.002 (2)	−0.018 (3)	−0.013 (3)
C14	0.115 (6)	0.102 (5)	0.054 (4)	−0.060 (4)	−0.007 (4)	−0.033 (4)
S2	0.0355 (6)	0.0263 (6)	0.0487 (7)	0.0013 (5)	−0.0126 (5)	−0.0151 (5)

O4	0.0537 (19)	0.0255 (16)	0.0522 (19)	0.0075 (14)	−0.0178 (16)	−0.0156 (15)
C15	0.066 (3)	0.039 (3)	0.057 (3)	0.010 (2)	−0.009 (3)	−0.026 (3)
C16	0.050 (3)	0.037 (3)	0.049 (3)	0.004 (2)	−0.017 (2)	−0.015 (2)
O5	0.062 (2)	0.0375 (19)	0.061 (2)	0.0060 (16)	−0.0097 (18)	−0.0177 (17)

Geometric parameters (Å, °)

Cu1—O3	2.019 (3)	C9—C10	1.398 (6)
Cu1—N2	2.059 (3)	C9—H9	0.9300
Cu1—N1	2.062 (3)	C10—H10	0.9300
Cu1—Cl1	2.2894 (13)	C11—C12	1.482 (5)
Cu1—Cl2	2.5390 (13)	S1—O3	1.557 (3)
O1—C5	1.222 (5)	S1—C13	1.776 (5)
O2—C6	1.230 (5)	S1—C14	1.785 (5)
N1—C12	1.356 (5)	C13—H13A	0.9600
N1—C1	1.358 (5)	C13—H13B	0.9600
N2—C10	1.351 (5)	C13—H13C	0.9600
N2—C11	1.357 (5)	C14—H14A	0.9600
C1—C2	1.398 (6)	C14—H14B	0.9600
C1—H1	0.9300	C14—H14C	0.9600
C2—C3	1.390 (6)	S2—O4	1.528 (3)
C2—H2	0.9300	S2—C16	1.798 (5)
C3—C4	1.406 (6)	S2—C15	1.802 (5)
C3—H3	0.9300	C15—H15A	0.9600
C4—C12	1.407 (5)	C15—H15B	0.9600
C4—C5	1.499 (6)	C15—H15C	0.9600
C5—C6	1.547 (6)	C16—H16A	0.9600
C6—C7	1.500 (6)	C16—H16B	0.9600
C7—C8	1.407 (6)	C16—H16C	0.9600
C7—C11	1.416 (5)	O5—H5A	0.9690
C8—C9	1.385 (6)	O5—H5B	0.9055
C8—H8	0.9300		
O3—Cu1—N2	164.67 (12)	C10—C9—H9	120.4
O3—Cu1—N1	88.13 (12)	N2—C10—C9	122.5 (4)
N2—Cu1—N1	80.35 (12)	N2—C10—H10	118.7
O3—Cu1—Cl1	92.68 (9)	C9—C10—H10	118.7
N2—Cu1—Cl1	93.81 (9)	N2—C11—C7	121.9 (3)
N1—Cu1—Cl1	156.11 (10)	N2—C11—C12	116.5 (3)
O3—Cu1—Cl2	95.00 (9)	C7—C11—C12	121.6 (3)
N2—Cu1—Cl2	96.66 (9)	N1—C12—C4	122.9 (3)
N1—Cu1—Cl2	98.39 (10)	N1—C12—C11	114.9 (3)
Cl1—Cu1—Cl2	105.31 (5)	C4—C12—C11	122.2 (3)
C12—N1—C1	117.9 (3)	O3—S1—C13	104.4 (2)
C12—N1—Cu1	114.5 (2)	O3—S1—C14	104.6 (2)
C1—N1—Cu1	127.5 (3)	C13—S1—C14	100.2 (4)
C10—N2—C11	118.8 (3)	S1—O3—Cu1	115.78 (16)
C10—N2—Cu1	127.5 (3)	S1—C13—H13A	109.5
C11—N2—Cu1	113.6 (2)	S1—C13—H13B	109.5
N1—C1—C2	122.7 (4)	H13A—C13—H13B	109.5

N1—C1—H1	118.6	S1—C13—H13C	109.5
C2—C1—H1	118.6	H13A—C13—H13C	109.5
C3—C2—C1	119.1 (4)	H13B—C13—H13C	109.5
C3—C2—H2	120.5	S1—C14—H14A	109.5
C1—C2—H2	120.5	S1—C14—H14B	109.5
C2—C3—C4	119.2 (4)	H14A—C14—H14B	109.5
C2—C3—H3	120.4	S1—C14—H14C	109.5
C4—C3—H3	120.4	H14A—C14—H14C	109.5
C3—C4—C12	118.2 (4)	H14B—C14—H14C	109.5
C3—C4—C5	121.9 (4)	O4—S2—C16	106.1 (2)
C12—C4—C5	119.9 (3)	O4—S2—C15	105.4 (2)
O1—C5—C4	122.8 (4)	C16—S2—C15	99.5 (2)
O1—C5—C6	119.3 (4)	S2—C15—H15A	109.5
C4—C5—C6	117.9 (3)	S2—C15—H15B	109.5
O2—C6—C7	122.0 (4)	H15A—C15—H15B	109.5
O2—C6—C5	119.0 (4)	S2—C15—H15C	109.5
C7—C6—C5	118.9 (4)	H15A—C15—H15C	109.5
C8—C7—C11	118.3 (4)	H15B—C15—H15C	109.5
C8—C7—C6	122.3 (4)	S2—C16—H16A	109.5
C11—C7—C6	119.4 (4)	S2—C16—H16B	109.5
C9—C8—C7	119.3 (4)	H16A—C16—H16B	109.5
C9—C8—H8	120.3	S2—C16—H16C	109.5
C7—C8—H8	120.3	H16A—C16—H16C	109.5
C8—C9—C10	119.2 (4)	H16B—C16—H16C	109.5
C8—C9—H9	120.4	H5A—O5—H5B	114.7
O3—Cu1—N1—C12	172.2 (3)	C5—C6—C7—C11	1.1 (6)
N2—Cu1—N1—C12	2.4 (3)	C11—C7—C8—C9	0.2 (6)
Cl1—Cu1—N1—C12	79.8 (4)	C6—C7—C8—C9	−177.2 (4)
Cl2—Cu1—N1—C12	−93.0 (3)	C7—C8—C9—C10	−1.4 (6)
O3—Cu1—N1—C1	−11.7 (3)	C11—N2—C10—C9	−0.2 (6)
N2—Cu1—N1—C1	178.5 (4)	Cu1—N2—C10—C9	176.0 (3)
Cl1—Cu1—N1—C1	−104.1 (4)	C8—C9—C10—N2	1.4 (6)
Cl2—Cu1—N1—C1	83.1 (3)	C10—N2—C11—C7	−1.0 (5)
O3—Cu1—N2—C10	139.4 (4)	Cu1—N2—C11—C7	−177.7 (3)
N1—Cu1—N2—C10	−178.8 (3)	C10—N2—C11—C12	178.8 (3)
Cl1—Cu1—N2—C10	24.6 (3)	Cu1—N2—C11—C12	2.1 (4)
Cl2—Cu1—N2—C10	−81.3 (3)	C8—C7—C11—N2	1.0 (6)
O3—Cu1—N2—C11	−44.2 (6)	C6—C7—C11—N2	178.5 (3)
N1—Cu1—N2—C11	−2.4 (2)	C8—C7—C11—C12	−178.8 (3)
Cl1—Cu1—N2—C11	−159.1 (2)	C6—C7—C11—C12	−1.3 (6)
Cl2—Cu1—N2—C11	95.0 (2)	C1—N1—C12—C4	0.1 (6)
C12—N1—C1—C2	−0.5 (6)	Cu1—N1—C12—C4	176.6 (3)
Cu1—N1—C1—C2	−176.5 (3)	C1—N1—C12—C11	−178.5 (3)
N1—C1—C2—C3	0.9 (7)	Cu1—N1—C12—C11	−2.0 (4)
C1—C2—C3—C4	−0.8 (7)	C3—C4—C12—N1	−0.1 (6)
C2—C3—C4—C12	0.5 (6)	C5—C4—C12—N1	−179.1 (3)
C2—C3—C4—C5	179.4 (4)	C3—C4—C12—C11	178.4 (4)
C3—C4—C5—O1	0.2 (6)	C5—C4—C12—C11	−0.6 (5)
C12—C4—C5—O1	179.1 (4)	N2—C11—C12—N1	−0.1 (5)

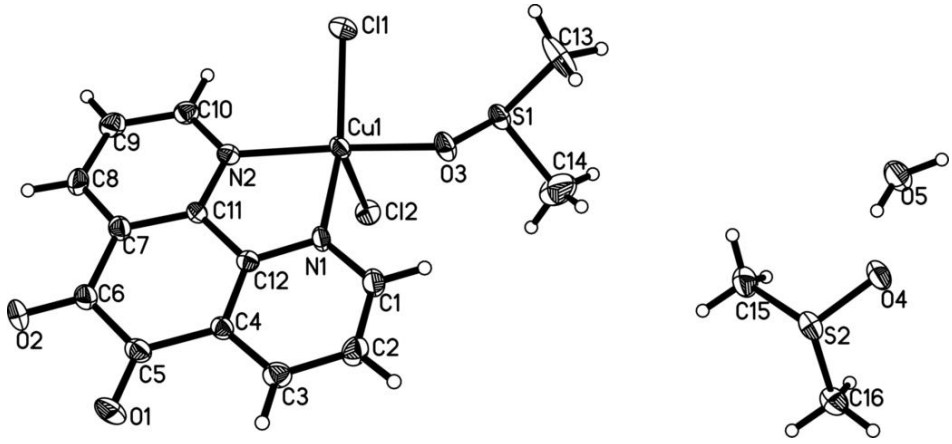
C3—C4—C5—C6	−178.6 (4)	C7—C11—C12—N1	179.7 (3)
C12—C4—C5—C6	0.4 (5)	N2—C11—C12—C4	−178.7 (3)
O1—C5—C6—O2	−0.8 (6)	C7—C11—C12—C4	1.1 (6)
C4—C5—C6—O2	178.0 (4)	C13—S1—O3—Cu1	135.8 (3)
O1—C5—C6—C7	−179.4 (4)	C14—S1—O3—Cu1	−119.4 (3)
C4—C5—C6—C7	−0.6 (6)	N2—Cu1—O3—S1	−168.1 (4)
O2—C6—C7—C8	−0.1 (6)	N1—Cu1—O3—S1	150.76 (19)
C5—C6—C7—C8	178.5 (4)	Cl1—Cu1—O3—S1	−53.13 (18)
O2—C6—C7—C11	−177.5 (4)	Cl2—Cu1—O3—S1	52.50 (18)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5A···O4	0.97	2.15	3.037 (5)	151
O5—H5B···Cl2^{i}	0.91	2.38	3.233 (5)	158

Symmetry codes: (i) *x*, *y*+1, *z*.

Fig. 1


Cl1
C13
C10
Cu1
S1
C9
N2
O3
C14
C8
C11
Cl2
O5
C7
C12
N1
C6
C1
C15
O4
C4
O2
C2
S2
C5
C3
C16
O1